

Application No. 09/696,071

RD-28030

AMENDMENTS TO THE CLAIMS:

This listing of claims will replace all prior versions and listings of claims in the application:

1. (currently amended) A method, comprising:

(A) defining a first experimental space comprising factors of at least two mixtures with at least one common factor;

~~(B) defining a second experimental space by deleting duplicate factor combinations from said first experimental space wherein said second experimental space is a ternary space comprising a number of experiments defined by determining a number of experiments for a succeeding experimental space by the relationship~~

$$V + \prod_{i=1}^3 n_i \times I_3 + \left[\sum_{i=1}^3 \frac{1}{n_i} \prod_{i=1}^3 n_i \right] \times I_2 \quad ;$$

for a ternary system ($T=3$) or an algorithm for a succeeding T -nary system, determined from a previous term by: (a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit higher than the first summation; (b) decrementing the subscript on I_i and (c) adding a value of n_i , indexed by the next index, to the inverse term;

(C) deleting duplicate factor combinations from the first determined experimental space to define a succeeding experimental space with a number of experiments determined in (B); and

~~(E)~~ (D) conducting a combinatorial high throughput screening (CHTS) experiment on said ~~second~~ succeeding experimental space, comprising an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating said identified products

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after completion of a single or repeated iteration ~~space~~ to select a best case set of factors from said second experimental space.

2. (canceled)

3. (canceled)

4. (canceled)

5. (canceled)

6. (canceled)

7. (currently amended) The method of claim 1, wherein said ~~second~~ succeeding experimental space factors comprise reactants, catalysts and conditions and said ~~(C)~~ (D) comprises (a) reacting a reactant selected from the ~~second~~ succeeding experimental space under a set of catalysts or reaction conditions selected from the ~~second~~ succeeding experimental space and (b) evaluating a set of products of the reacting step and further comprising ~~(D)~~ (E) reiterating step ~~(C)~~ (D) wherein a next ~~second~~ succeeding experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step ~~(C)~~ (D).

8. (currently amended) The method of claim 7, comprising reiterating ~~(C)~~ (D) until a best set of factors of said second experimental space is selected.

9. The method of claim 1, wherein said first experimental space includes a catalyst system comprising combinations of Group IVB, Group VIB and Lanthanide Group metal complexes.

10. (currently amended) The method of claim 1, wherein said ~~second~~ succeeding experimental space includes a catalyst system comprising a Group VIII B metal.

11. (currently amended) The method of claim 1, wherein said ~~second~~ succeeding experimental space includes a catalyst system comprising palladium.

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12. (currently amended) The method of claim 1, wherein said ~~second~~ succeeding space includes a catalyst system comprising a halide composition.

13. (currently amended) The method of claim 1, wherein said ~~second~~ succeeding experimental space includes an inorganic co-catalyst.

14. (currently amended) The method of claim 1, wherein said ~~second~~ succeeding experimental space includes a catalyst system that includes a combination of inorganic co-catalysts.

15. (canceled)

16. (canceled)

17. (canceled)

18. (currently amended) A system for selecting a best case set of experiments of a experimental reaction, comprising;

a processor that (A) defines a first experimental space comprising factors of at least two mixtures with at least one common factor; and (B) ~~defines a second experimental space by deleting duplicate factor combinations from said first experimental space and wherein said second experimental space is a ternary space comprising a number of experiments defined by~~ determines a number of experiments for a succeeding experimental space by the relationship

$$V + \prod_{i=1}^3 n_i \times I_3 + \left[\sum_{i=1}^3 \frac{1}{n_i} \prod_{i=1}^3 n_i \right] \times I_2$$

for a ternary system ($T=3$) or an algorithm for a succeeding T -nary system, determined from a previous term by: (a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit higher than the first summation; (b) decrementing the subscript on I_i and (c) adding a value of n_i , indexed by the next index, to the inverse term; and (C) deletes duplicate factor combinations from the first determined experimental space to define a succeeding experimental space with a

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number of experiments determined in (B); and

a reactor and evaluator to select a best case set of factors from said succeeding experimental space by a combinatorial high throughput screening (CHTS) method to select a best case set of factors from said experimental space.

19. The system of claim 18, wherein said processor comprises

a display terminal having screen displays whereby a researcher can input values for factors on said screen;

a database for storing said factors;

a computer for generating a set of test cases for a set of said factors based on a researcher specified value for identifying a number of interacting relationships within said factors;

a computer combining said test cases for set of factors with said relationships and providing a merged table of test cases; and

an output for writing to a database said merged table of test cases.

20. (canceled)

21. (currently amended) The system of claim 18, wherein said ~~second~~ succeeding experimental space is a quaternary space comprising a number of experiments defined by

$$V + \prod_{i=1}^4 n_i \times I_4 + \left[\sum_{i=1}^4 \frac{1}{n_i} \prod_{i=1}^4 n_i \right] \times I_3 + \left[\sum_{i=1}^4 \sum_{j=1}^4 \frac{1}{n_i n_j} \prod_{i=1}^4 n_i \right] \times I_2$$

22. The system of claim 18, wherein said ~~second~~ succeeding experimental space is a pentanary space comprising a number of experiments defined by

$$V + \prod_{i=1}^5 n_i \times I_5 + \left[\sum_{i=1}^5 \frac{1}{n_i} \prod_{i=1}^5 n_i \right] \times I_4 +$$

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$$\left[\sum_{i=1}^5 \sum_{j=i+1}^5 \frac{1}{n_i n_j} \prod_{i=1}^5 n_i \right] \times I_3 + \left[\sum_{i=1}^5 \sum_{j=i+1}^5 \sum_{k=j+1}^5 \frac{1}{n_i n_j n_k} \prod_{i=1}^5 n_i \right] \times I_2.$$

23. An experimental space, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^T n_i \times I_T + \left(\sum_{i=1}^T \frac{1}{n_i} \right) \times \left(\prod_{i=1}^T n_i \right) \times [I_{(T-1)}]$$

for a ternary system ($T = 3$) or an algorithm for a succeeding T -nary system, determined from a previous term by: (a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit higher than the first summation; (b) decrementing the subscript on I ; and (c) adding a value of n , indexed by the next index, to the inverse term.

24. The experimental space of claim 23, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^4 n_i \times I_4 + \left[\sum_{i=1}^4 \frac{1}{n_i} \prod_{i=1}^4 n_i \right] \times I_3 + \left[\sum_{i=1}^4 \sum_{j=i+1}^4 \frac{1}{n_i n_j} \prod_{i=1}^4 n_i \right] \times I_2$$

for a quaternary system.

25. The experimental space of claim 23, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^5 n_i \times I_5 + \left[\sum_{i=1}^5 \frac{1}{n_i} \prod_{i=1}^5 n_i \right] \times I_4 + \left[\sum_{i=1}^5 \sum_{j=i+1}^5 \frac{1}{n_i n_j} \prod_{i=1}^5 n_i \right] \times I_3 + \left[\sum_{i=1}^5 \sum_{j=i+1}^5 \sum_{k=j+1}^5 \frac{1}{n_i n_j n_k} \prod_{i=1}^5 n_i \right] \times I_2$$

for a pentanary system.